Electronic Supplementary Material (ESI) for RSC Advances

SUPPORTING INFORMATION

Electron Detachment Dynamics of $O_2^-(H_2O)$:

Direct Ab initio Molecular Dynamics (AIMD) Approach

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1. Electron detachment dynamics of $O_2^-(H_2O)$ with C2v symmetry.

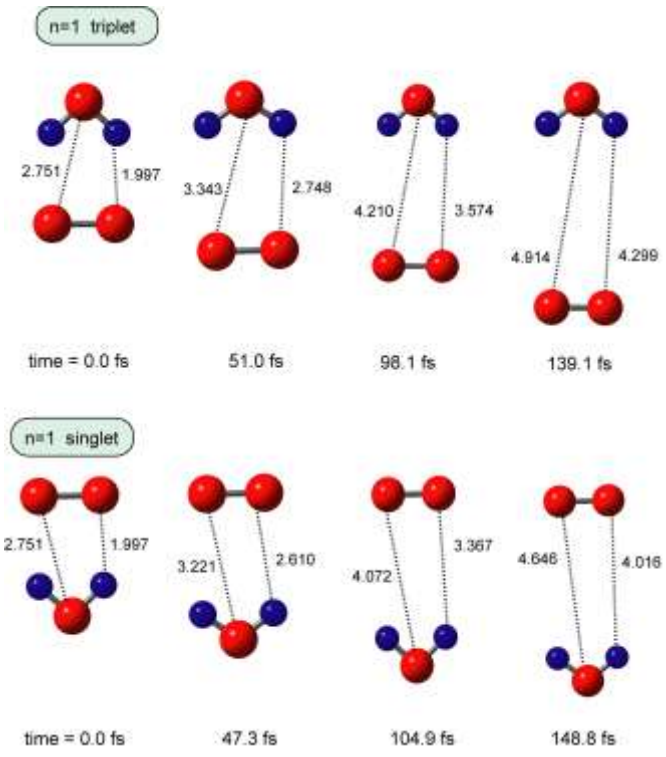

Figure S1. Electron detachment dynamics of $O_2^-(H_2O)$ with C_{2v} on ***triplet*** and ***singlet*** potential energy surfaces. The values indicate intermolecular distances (in Å). Dynamics calculation were carried out at the MP2/6-311++G(d,p) level. The trajectory was started from the optimized geometry of $O_2^-(H_2O)$ with C_{2v} structure.

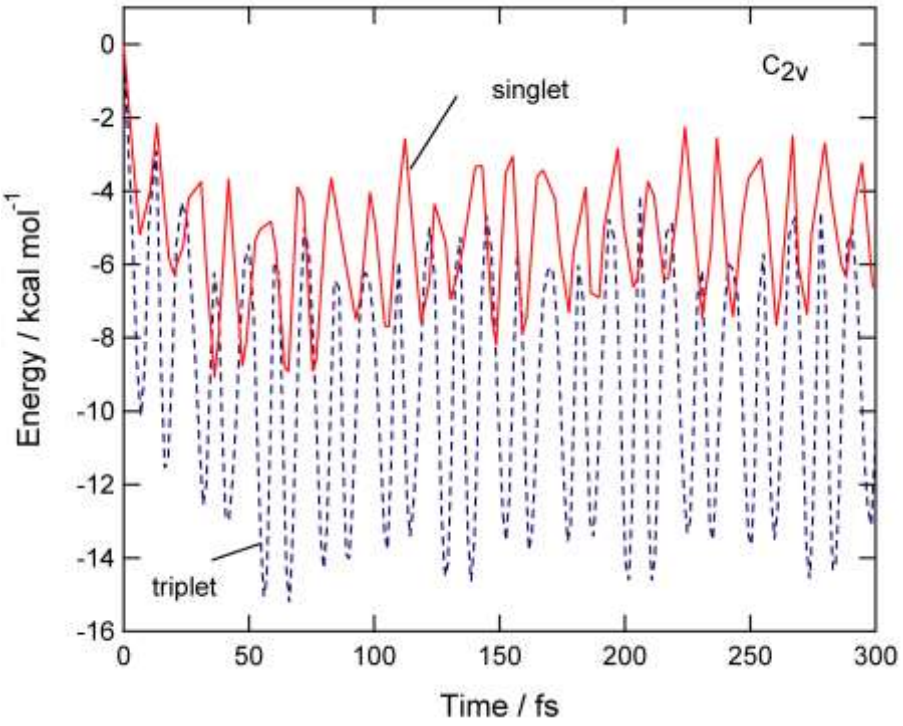

Figure S2. Time evolutions of potential energies of $O_2(H_2O)$ on singlet and triplet state PESs.

2. Effects of initial structures on the reaction dynamics.

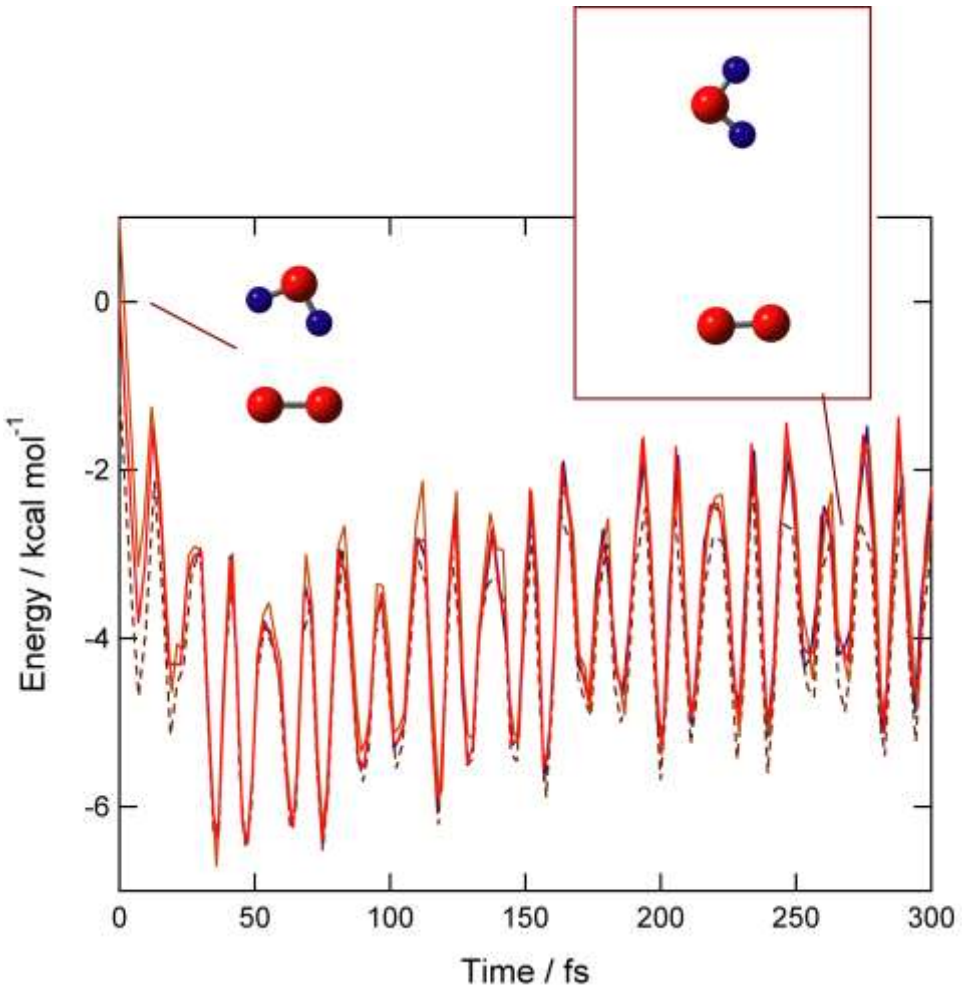

Figure 3. Effects of initial configurations on the time evolutions of potential energies of $O_2(H_2O)$ on singlet state PES.